

4-Aminofluorene

Inchi:	InChI=1S/C13H11N/c14-12-7-3-5-10-8-9-4-1-2-6-11(9)13(10)12/h1-7H,8,14H2
InchiKey:	NNHRVRJFHLVIIV-UHFFFAOYSA-N
Formula:	C13H11N
SMILES:	Nc1cccc2c1-c1ccccc1C2
Mol. weight [g/mol]:	181.23
CAS:	7083-63-8

Physical Properties

Property code	Value	Unit	Source
gf	413.62	kJ/mol	Joback Method
hf	266.25	kJ/mol	Joback Method
hfus	22.80	kJ/mol	Joback Method
hvap	61.59	kJ/mol	Joback Method
ie	7.60	eV	NIST Webbook
ie	7.25	eV	NIST Webbook
log10ws	-4.05		Crippen Method
logp	2.840		Crippen Method
mcvol	145.630	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	325.11		NIST Webbook
tb	640.54	K	Joback Method
tc	896.04	K	Joback Method
tf	439.15	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.54	J/mol×K	640.54	Joback Method
cpg	374.87	J/mol×K	683.12	Joback Method
cpg	387.10	J/mol×K	725.71	Joback Method
cpg	398.37	J/mol×K	768.29	Joback Method
cpg	408.83	J/mol×K	810.88	Joback Method
cpg	418.63	J/mol×K	853.46	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7083638&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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